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RESEARCH ARTICLE

ESTIMATING OPTIMUM PROPERTIES USING ENUMERATED DATA BY MATLAB FOR CALCIUM CARBONATE/PP NANOCOMPOSITES AS BONE ANALOGUE BIO COMPOSITE

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ABSTRACT

This paper present modified polymer matrix bio composite for bone analogue and replacement. Using PP polymer as polymeric matrix give robust properties especially when used with Nano ceramic filler. Nano CaCO3 and Al2O3 proposed in this work as a filer, the optimum processing conditions for Calcium Carbonate/PP Nanocomposites as bone analogue biomaterials is sought using Enumerated data by MATLAB. Also the effect of nano sized Al_2O_3 on the mechanical properties was studied. ESM by MATLAB software, give an indication for optimum processing condition which are commensurate with classical experiments design. Different compositions, compounding pressure, and processing temperatures were used in this work. Composite with 5% Al_2O_3/20 CaCO3/75PP give the optimum mechanical properties and uniform distribution of fillers in polymeric matrix.

INTRODUCTION

Defects in bones, can arise duo to several causes such as trauma, infection, tumors, or bone diseases (i.e., osteoporosis), are very common in our society. Most therapies for bone defects are based on autografts or allografts. Autografts means that tissues are grafted in the same individual ,whileAllografts, "are the transplantation of tissue -in this case bone tissue- between genetically nonidentical individuals of the same species, are an attractive alternative to autografts.Bone allografts may be cancellous, cortical, or a combination of each; and it is possible to manufacture customized types, such as dowels, strips, and chips ". (Duan, B., *et al*, 2010) Many investigations was take place to develop biomaterial systems which can use to repair or replace natural bone just in case of complicated fracture , previous folks suffer from accidently fractures, and bone cancer patients (Bret D, *et al*, 2011) Biomaterials for bone repair and replacement ought to possess biocompatibility, lack of inflammation, biodegradation, besides to mechanical properties that ought to be near natural bone properties. At present, bone grafts and replacement poses challengeto develop biomaterialsfor scaffold applications.

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This might be achieved via any of either endogenous or exogenous materials: auto graft, allograft or a xenograft (Kashan, Jenan, S, *et al*, 2016). During last decades, most orthopedical implants were made of metallic materials, these including, but not limiting to γ- stainless steel, Co-Cr and Ti-alloys, due to their superior strength, toughness, and good ductility. Anyway, modulus of elasticity (*E*) of such alloys extremely higher than that of human bones. This creates a stress shielding effect of the surrounding bone tissue, causing the implant to carry a higher proportion of the applied load (Hallab, *et al*,2001). Moreover, human body fluids with0.9 wt% NaCl salt content at 37 °C, are hostile to metallic alloys. Thus, metallic implants may undergo dissolution or corrosion upon exposure to human body fluids, releasing metallic ions that induce an inflammatory response, allergy, and cytotoxicity. (Scharf, *et al*, 2014). Polymers have useful applications in scaffold application, due to their good biocompatibility, less of inflammation. Moreover, lightweight, the ease of fabrication and the relatively low cost. Their tensile stress and modulus can be modified by adding fillers of micrometer or Nano sizes. Moreover, some polymers can be act as the natural collagen in natural bone like HDPE, PP, and PLA, but there is a Lake of strength and wear. This inspired researchers to use the composite approach which is an effective route for producing polymer biomaterials with desired mechanical properties for bone replacements (Tjong, *et al*, 2000). CaCO3 consider one of the most commonly used fillers in thermoplastics because it is inexpensive, and can be used at high loadings (Gorna K., *et al*, 2008). Now, CaCO3 is being produced in Nano meter size, thisNano precipitated CaCO3 (NPCC) has the potential to be a crucial practical filler in plastic composites (Liang, 2007, Chiba, *et al*, 2003). To improve mechanical properties for compound biocompsite, bio inert ceramic compound is also utilized in sufficient amounts to boost mechanical properties for implants that possess appropriate properties among acceptable values to avoid stress shielding. Hence, ceramic oxides or metallic dispersions are introduced as reinforcing agent. Among the ceramic reinforcement, alpha- Al2O3 has been utilized in orthopedically application because of its glorious wear resistance. (Duncan, 2011). Recently, advances in nanotechnology have led to the development and many functional Nanomaterials with unique characteristics, Which nominate the use of Nanomaterials in healthcare and biomedical applications (Hule *et al.*, 2007, Zhang, *et al.*, 2009). One of the most important issue to be considered in suggested biomaterials for bone autograft and allograft, is their mechanical properties and their distribution within prepared biomaterial, so that several optimization methods can be adopted to In the present study, Calcium Carbonate/PP Nanocomposites was synthesis for orthopedic application. Alumina used in nano size to modify mechanical properties for implants. MATLAP software have used to optimize mechanical properties measured within mechanical testing for implants.

EXPERIMENTAL

MATERIALS AND METHODS

Right Fortune Industrial restricted (Shanghai, China) provided PP powder with average particle size of 10 nm and a nominal density of 0.911 g/cm3 used for this study. Nano CaCO3powder with ninety nine purity, having an average particle size of 20nm and a particle density of 2.93 g.cm^{-3}, and α-alumina powder withaverage particle size of 40nm and density of 3.97 g.cm^{-3}, were used as ceramic fillers. Ceramic powders were provided by provided by M.K. Nano (Toronto, Canada).

Preparation of Nanocomposites

Ball mill dry mixing used to mix powders with different weight% (Table 1). Hot pressing technique used to prepare samples using hot pressing system designed especially for this study, different compression pressure and compounding temperatures were used Table 1.

Table 1. Sample preparation conditions

Composition(weight%)	Compression pressure(MPa)	Compounding temperature (C°)
10%$CaCO_3$+90% PP	30,60,90	180, 190,200
20% CaCO3 +80PP	30,60,90	180, 190,200
5%Al_2O_3+20% CaCO3 +75%PP	30,60,90	180, 190,200

Density and mechanical properties testing

Pycnometer instrument of sort AccuPyc1330 Pycnometer (AccuPyc from Micromeritics Instrument Corporation, Holland) wont to live bulk density for all samples, whereas fracture strength was calculated from diametrical compression take a look at mistreatment Instron tensile machine with a crosshead speed of five millimeter min-1.

Following formula wont to calculate fracture strength (Procopio, *et al*, 2003):

$\sigma f = 2P/\pi\ Dt$ ……………………..(1)

Where:
σf : Tensile fracture strength (MPa), P: Cross head load (N), D: Specimen diameter (mm), and t: Specimen thickness (mm). micro hardness values were calculated mistreatment micro hardness tester (Digital Micro-Vickers Hardness tester TH714) for national capital TIME engineering Ltd./China).

SEM Structure Analysis

LEO-SEM 1530 scanning microscopy has been wont to study the morphology of the samples was studied mistreatment, at an accelerating voltage voltage of 5kV and a operating distance of 6mm. The samples were secured onto specimen holders by conductive carbon cement and coated with 5 nm layer of Pd-Pt (20:80) by CVD technique. The imaging process was controlled using Smart SEM software.

Optimization Processusing Matlab Software

Enumerated data is data that is restricted to a finite set of values. An enumerated data type is a MATLAB® class that defines a set of enumerated values. Each enumerated value consists of an enumerated name and an underlying integer which the software uses internally and in generated code. (Joko, *et al*, 2015) Enumeration method test all possible solutions one by one, searching for an optimal solution.

This method lists all possible solutions and then eliminates the non-optimal schedules from the list, leaving those, which are optimal. The optimal criteria are considering by the decision makers. Clearly searching for an optimal solution among all possible solutions using complete enumeration is not suitable even for problems of small size (Kathiravan, Ganguli, 2007). MATLAB software used in this work to estimate optimum properties depending on processing condition. Moreover, strength/weight ration have calculated because in scaffold application, it is important to produce bone or scaffold with a balance between mechanical properties and suitable weight.

RESULTS AND DISCUSSION

Density and Mechanical Properties

Figures (1-3) shows the result of various process conditions on density and measured mechanical properties. Those figures listed attention-grabbing sweetening with increasing CaCO3wt.%, whereas samples with alumina content has superior properties and really near natural bone properties. (Tony and Wilson, 1993) Nano sized fillers affected completely on the mechanical properties, this finding is corresponding with the previous investigations (Kaviani and Zamanian, 2015, Hule, and Pochan, 2007).

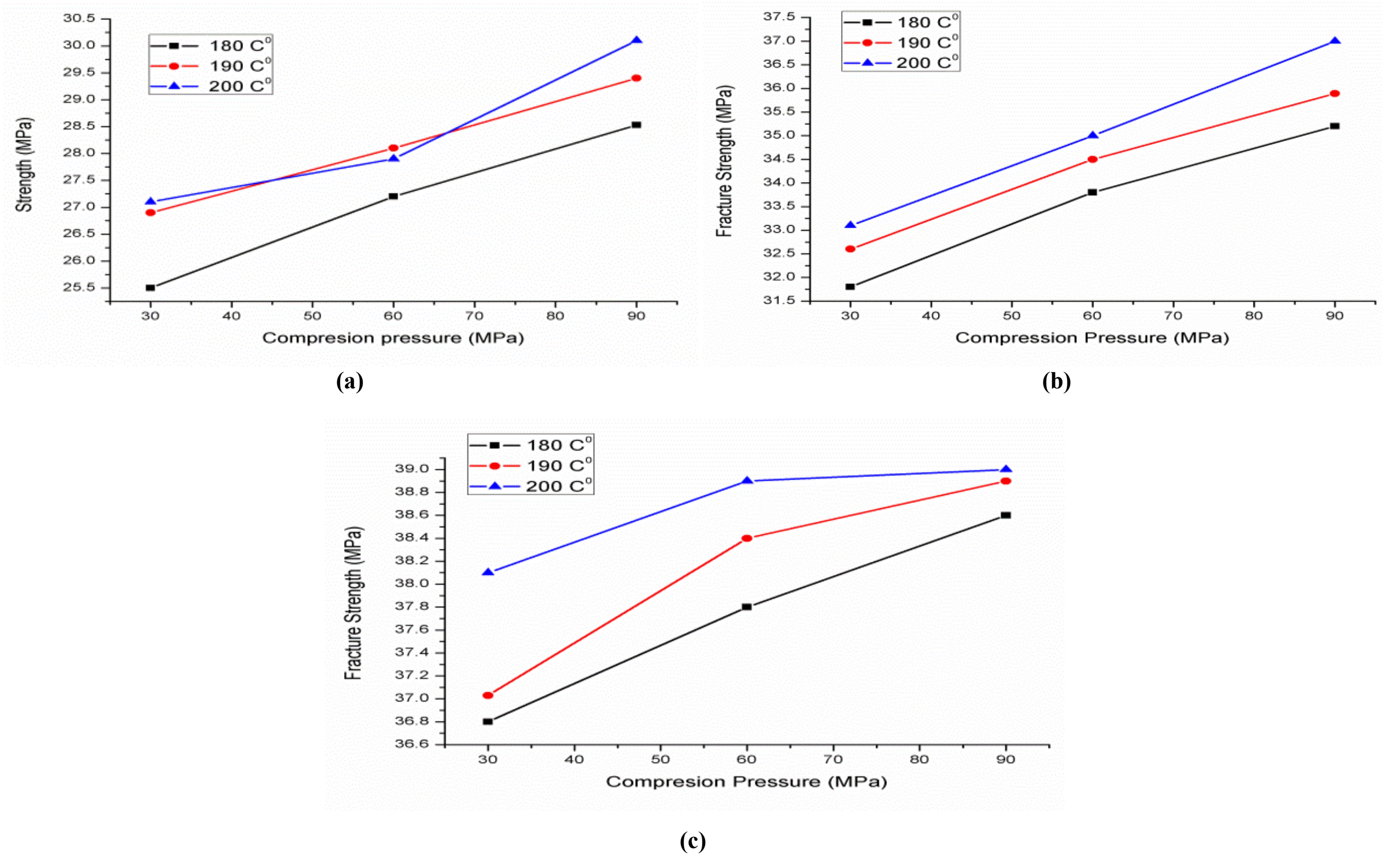


Figure 1. Relationship between compression pressure and fracture strength a) at 10 CaCO3 /90PP, b) 20CaCO3 /80PP, c)5Al203/20 CaCO3 /75PP

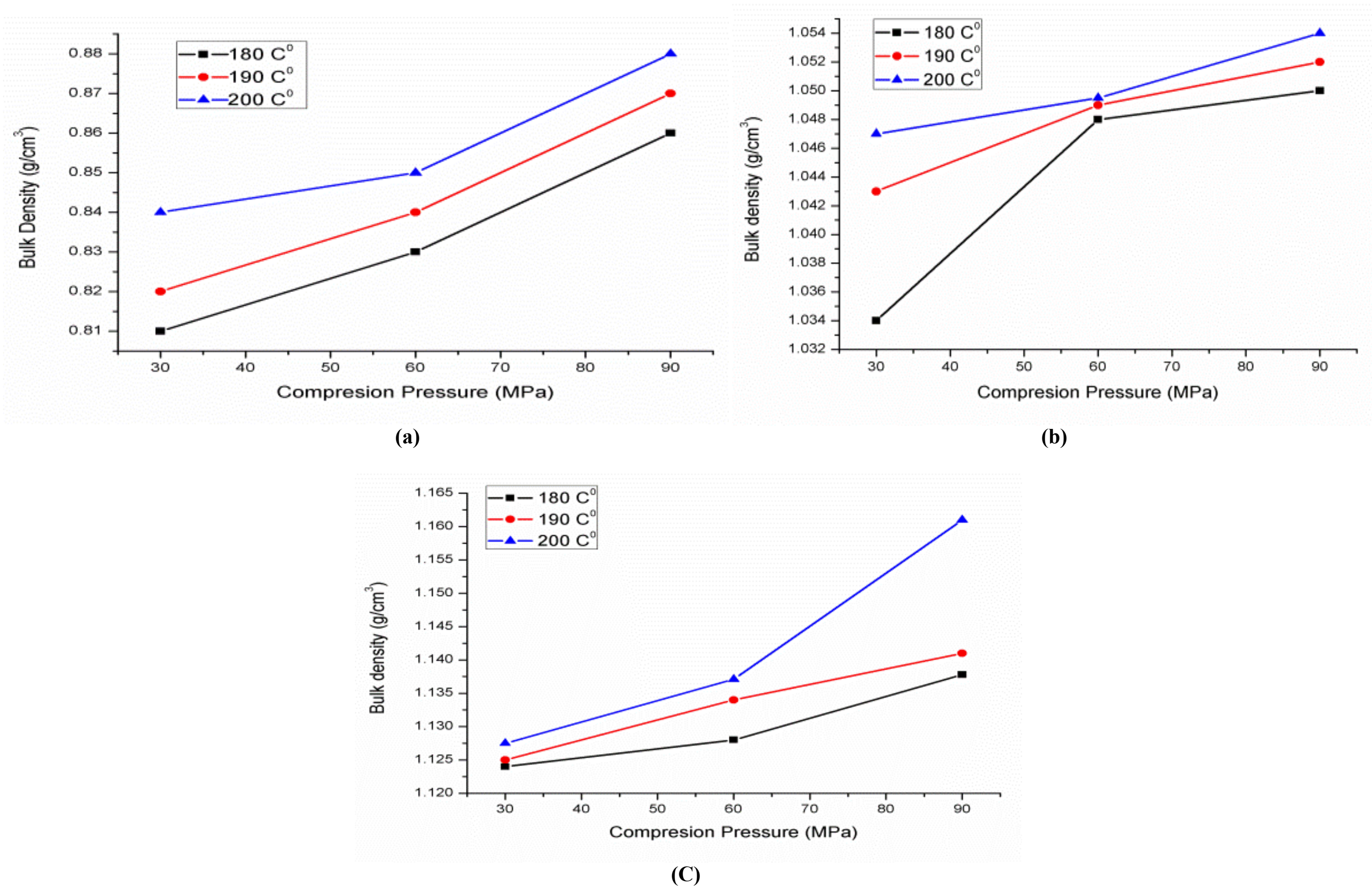
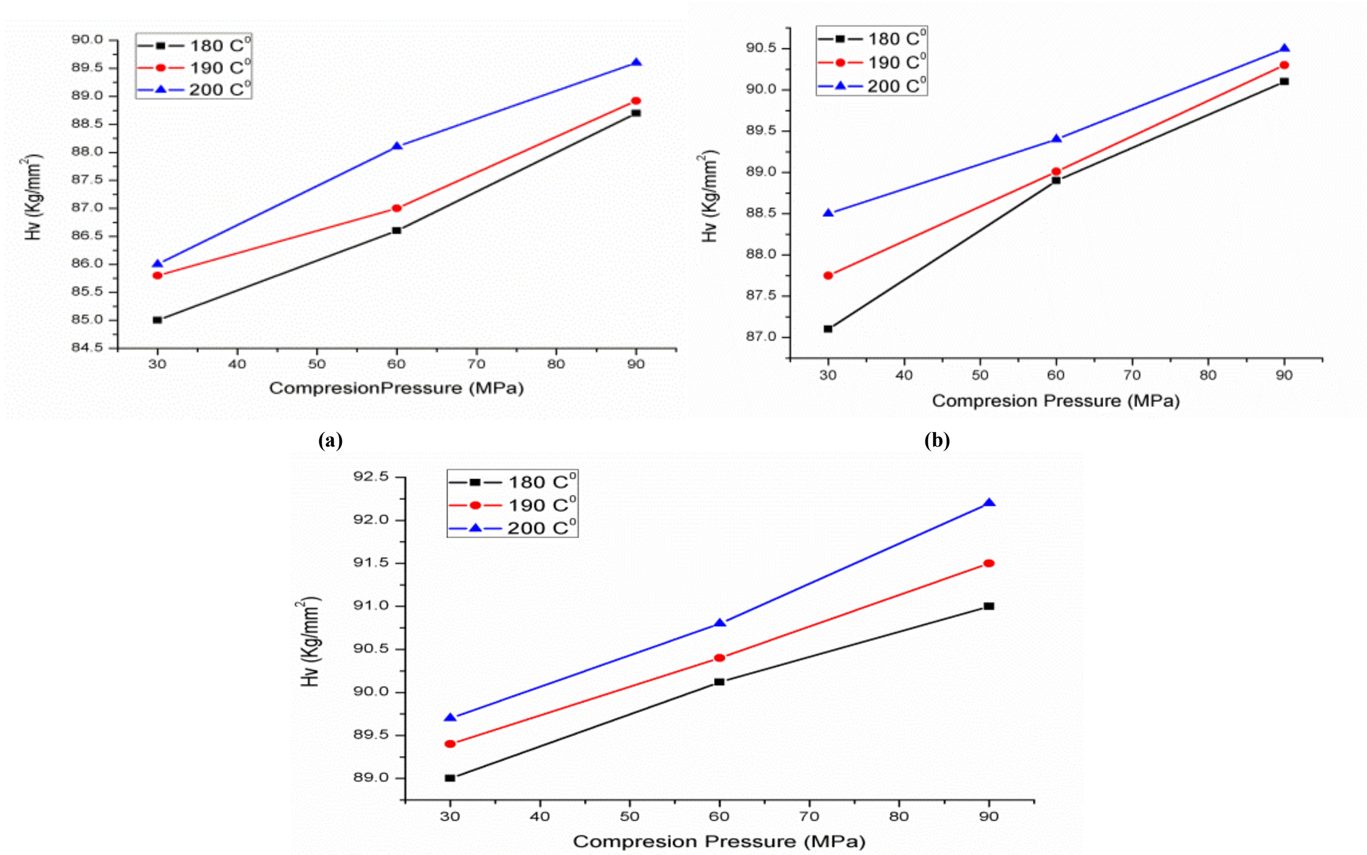


Figure 2. Relationship between compression pressure and Density a) at 10 CaCO3 /90PP, b) 20 CaCO3 /80PP, c) 5Al203/20 CaCO3 /75PP

composition 5Al2O3/20CaCO3/75PP, 20CaCO3/80PP, 10CaCO3/90PP from top to bottom layer. Figure (5) shows the same model but for hardness-temperature-pressure, while Figure(6) shows the above model but for strength-temperature-pressure. Figure (7) shows the mean value for all outputs, density have the lowest values in the curves as a comparison with hardness and strength values which are in the same level approximately.



(a) (b)

(c)

Figure 3. Relationship between compression pressure and microhardness a) at 10 CaCO3 /90PP, b) 20 CaCO3 /80PP, c) 5Al203/20 CaCO3 /75PP

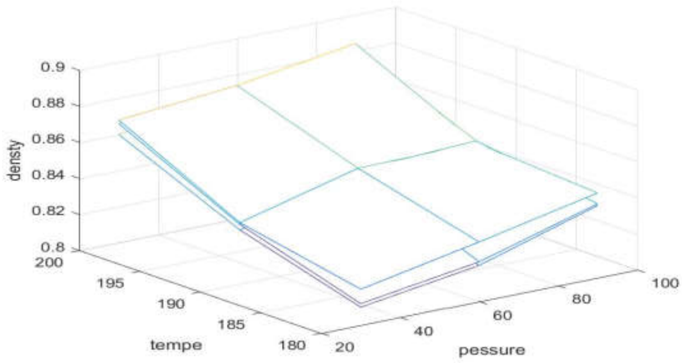


Figure 4. Density – Compounding Temperature-Compression Pressure ByMATLAB Enumeration method

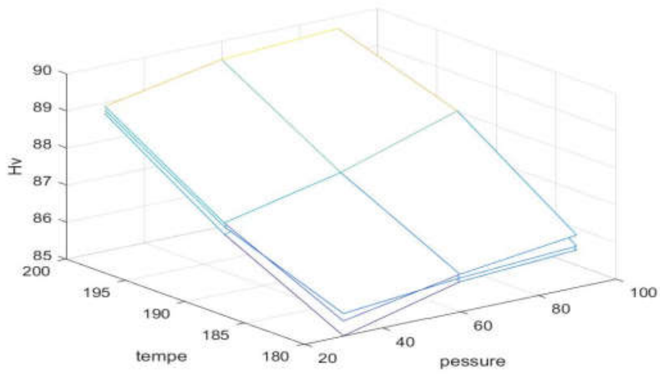


Figure 5. Hardness – Compounding Temperature-Compression Pressure ByMATLAB Enumeration method

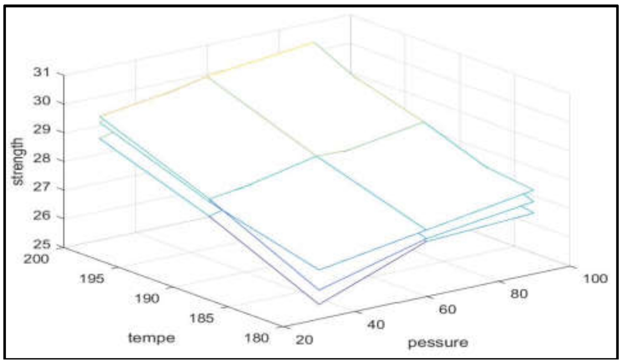


Figure 6. Fracture Strength – Compounding Temperature-Compression Pressure ByMATLAB Enumeration method

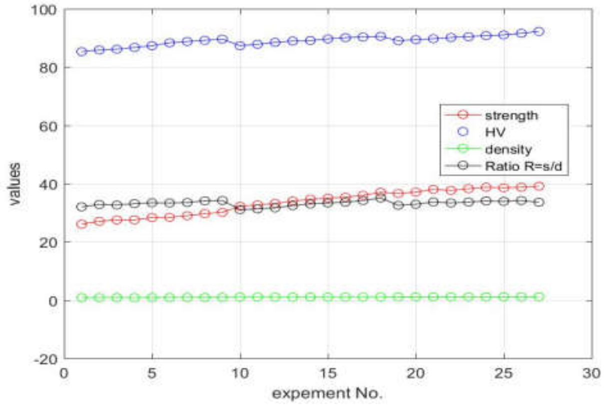
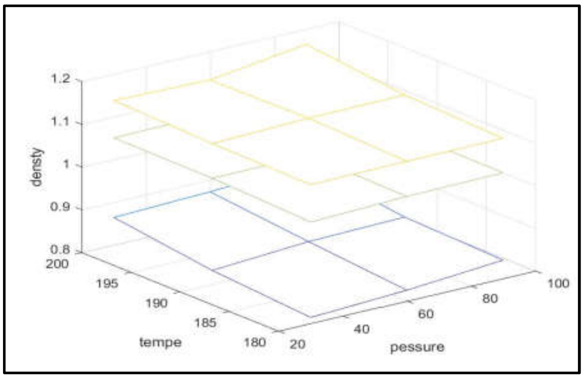
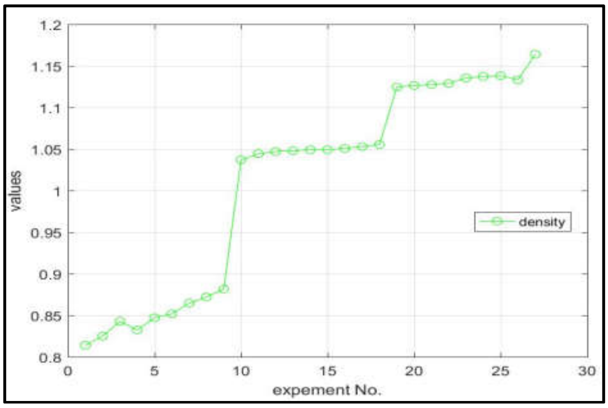


Figure 7. The mean value of all outputs By MATLAB Enumeration method



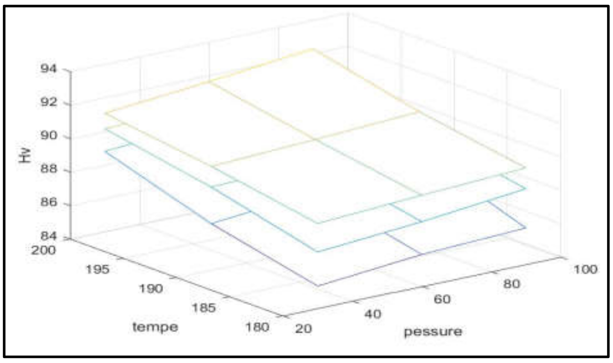
(a)



(b)

Figure 8. The mean value of Density a) 3D, each level corresponds to one composition, b) 2D, By MATLAB Enumeration method

The interesting curve belongs to strength/ density ratio which have the highest values, the implants that have a superior mechanical properties with suitable weight consider promising biomaterials for scaffolds especially for old aged people, (Zena, *et al*, 2015; Mour *et al*, 2010).



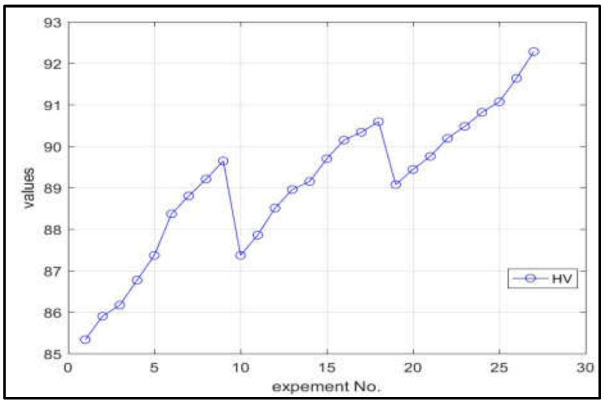
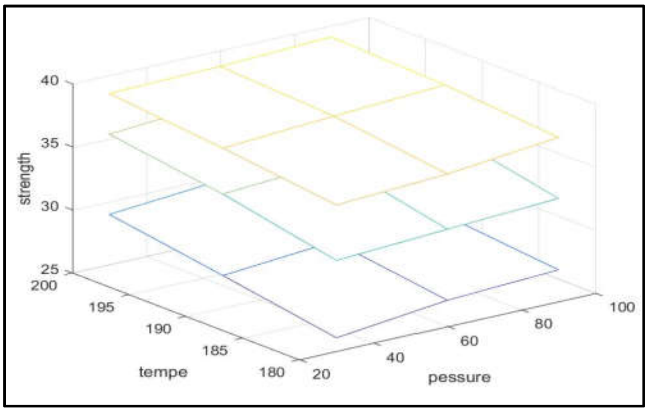


Figure 9. The mean value of Hazrdness a) 3D, each level corresponds to one composition, b) 2D, By MATLAB Enumeration method



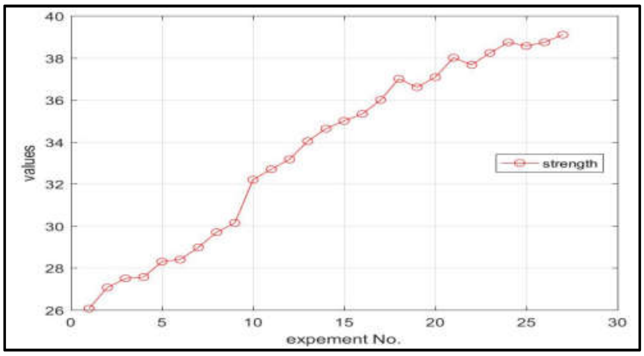
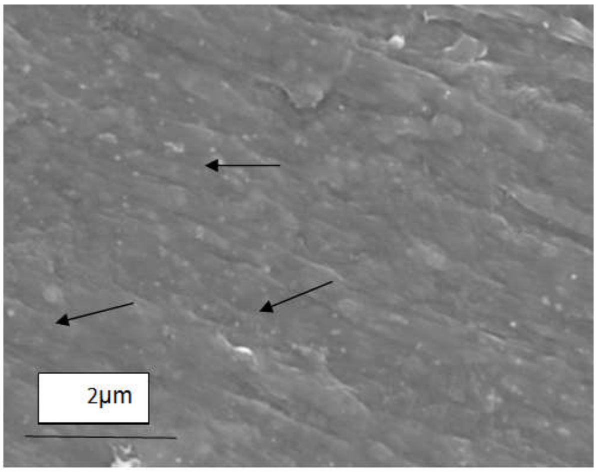
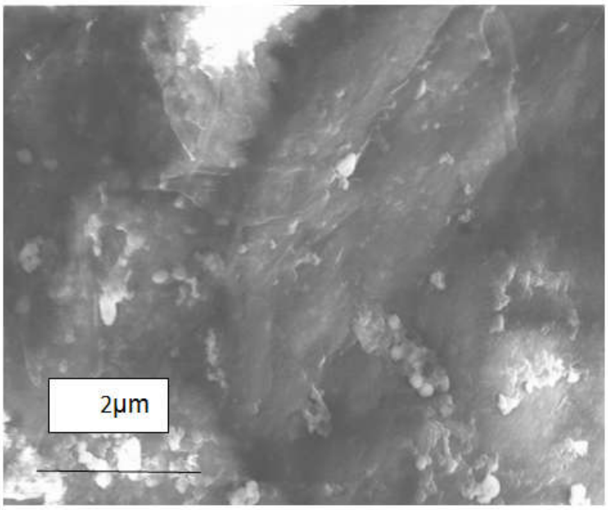


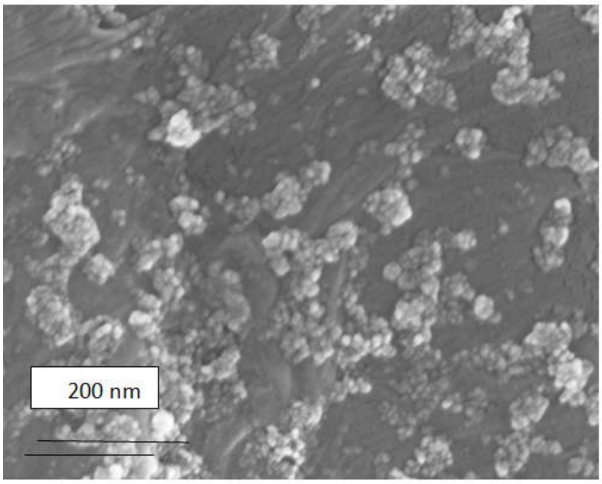
Figure 10. The mean value of Strength a) 3D, each level corresponds to one composition, b) 2D, By MATLAB Enumeration method



(a)



(b)



(c)

Figure 11. SEM a) 10 $CaCO_3$/90PP implant, b) 20 $CaCO_3$/80PP, c) 5Al_2O_3/20 $CaCO_3$/80PP all photos shows uniform distribution for Nano filler in polymer matrix

Figures (8-10) shows the mean value in 3D and 2D distribution for density, hardness, and strength respectively. For density, optimum values located between 1to 1.2, however these values indicate that optimum density within 5Al_2O_3/20$CaCO_3$/75PP composition layer. The same behaviour for both of hardness and strength results. From above, optimum conditions for implants available in the of5Al_2O_3/20$CaCO_3$/75PP.

Morphology

Figure 11 show a uniform distribution or Nano ceramic filler within polymeric matrix for all composition used in this work, Nano filler distributed as particles and small agglomerate in PP matrix which have good impact on mechanical properties for biocomposite materials subject of this investigation.

Conclusion

$CaCO_3$/PP Nano composite gives an interesting property for bone analogue and substitute application. The addition of alumina enhances mechanical properties for the composite materials but within suitable range. Polymeric matrix biocomposite investigated in this work can be biomimetic for natural bone. Enumeration method using MATLAB software considers an effective analysis tool when all possible results must take place in optimization process.

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Highlights

- Nano sized Alumina and Calcium Carbonate fillers effect on mechanical properties of PP polymeric matrix was investigated.
- Density, Microhardness, and fracture strength were characterized for 3 different compositions.
- Optimum Properties Using Enumerated data by MATLAB software were investigated.
- SEM used for morphology records.
- Optimum properties was very close to natural bone properties.

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